Rotundone

Inchi: InChI=1S/C15H22O/c1-9(2)12-6-5-10(3)15-13(8-12)11(4)7-14(15)16/h10-12H,1,5-8H2,2-
InchiKey: NUWMTBMCSQWPDG-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CCC(C)C2=C(C1)C(C)CC2=O
Mol. weight [g/mol]: 218.33
CAS: 18374-76-0

Physical Properties

Property code	Value	Unit	Source
gf	108.21	kJ/mol	Joback Method
hf	-239.53	kJ/mol	Joback Method
hfus	20.91	kJ/mol	Joback Method
hvap	54.46	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.904		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	1722.40		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1722.40		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
tb	641.99	K	Joback Method
tc	871.82	K	Joback Method
tf	354.67	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.27	J/mol×K	641.99	Joback Method
cpg	565.40	J/mol×K	680.30	Joback Method
cpg	586.17	J/mol×K	718.60	Joback Method

cpg	605.60	J/mol×K	756.91	Joback Method
cpg	623.72	J/mol×K	795.21	Joback Method
cpg	640.55	J/mol×K	833.52	Joback Method
cpg	656.12	J/mol×K	871.82	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18374760&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume